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L4 2842848 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR AMIN? OR PROTEOME?)

L5 224579 SEA FILE=HCAPLUS (MASS(W)SPECTR?)
L6 26790 SEA FILE=HCAPLUS L4(L)L5
L14 1924052 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR PROTEOME?)
L27 1886 SEA FILE=HCAPLUS L14 (W)MASS
L28 1074 SEA FILE=HCAPLUS L27 AND L6
L30 436 SEA FILE=HCAPLUS L28 AND IDENT?
L33 6258 SEA FILE=HCAPLUS L14(W)IDENT?
L34 115 SEA FILE=HCAPLUS L30 AND L33
L35 48 SEA FILE=HCAPLUS L34 NOT (2001 OR 2000 OR 1999)/PY

=> d ibib abs hitrn 135 1-48

L35 ANSWER 1 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1999:3528 HCAPLUS
DOCUMENT NUMBER: 130:150603
TITLE: Examination of micro-tip reversed-phase liquid chromatographic extraction of **peptide** pools for **mass spectrometric** analysis
AUTHOR(S): Erdjument-Bromage, Hediye; Lui, Mary; Lacomis, Lynne; Grewal, Anita; Annan, Roland S.; McNulty, Dean E.; Carr, Steven A.; Tempst, Paul
CORPORATE SOURCE: Molecular Biology Program, Memorial Sloan-Kettering

Cancer Center, New York, NY, 10021, USA
SOURCE: J. Chromatogr., A (1998), 826(2), 167-181
CODEN: JCRAEY; ISSN: 0021-9673
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB **Mass spectrometry** occupies a central position in most current **protein identification** schemes. So-called 'mass fingerprinting' techniques rely on composite mass patterns of proteolytic fragments, or dissocn. products thereof, to query databases. Keys to successful anal. of ever smaller amts. are sensitivity and complete spectral information, both of which depend for a large part on proper sample prepn. Clean-up and concn. of **peptide** mixts. over Eppendorf gel loading tips filled with chromatog. media (i.e. 'micro-tips') are believed to be quite useful in this regard. We have studied quant. and qual. aspects of **polypeptide** extn. using these small manual devices. Optimization of sample vol. and additives, micro-tip bed vol., and eluent compn. and vol., all contribute to effective recovery (.apprx.65-70%, on av.). Improper digest conditions can, in fact, lead to far bigger losses, suggesting the need for at least trace amts. of Zwittergent 3-16. Of particular interest is our finding that partial fractionation, obtained by two-step micro-tip elution, generally results in more and better signals during subsequent mass anal. Thus, by using optimized micro-tips, in combination with adequate sample handling and instrumentation, direct **mass spectrometric identification** can be routinely and successfully done in any resource facility type setting.

REFERENCE COUNT: 29
REFERENCE(S):
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(7) Eng, J; J Am Soc Mass Spectrom 1994, V5, P976 HCAPLUS
(8) Erdjument-Bromage, H; Techniques in Protein Chemistry IV 1993, P419 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 2 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:785231 HCAPLUS
DOCUMENT NUMBER: 130:121579
TITLE: **Mass spectrometric identification** and microcharacterization of **proteins** from electrophoretic gels: strategies and applications
AUTHOR(S): Jensen, Ole Norregaard; Larsen, Martin R.; Roepstorff, Peter
CORPORATE SOURCE: Department of Molecular Biology, Odense University, Odense, Den.
SOURCE: Proteins: Struct., Funct., Genet. (1998), (Suppl. 2), 74-89
CODEN: PSFGEY; ISSN: 0887-3585
PUBLISHER: Wiley-Liss, Inc.

DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 77 refs. including the authors' own research. The entire genomic DNA sequences of a no. of prokaryotic and eukaryotic species are now available and many more, including the human genome, will be completed in the near future. The state-of-life of a cell at any given time, however, is defined by its **protein** compn., i.e., its **proteome**. Gel electrophoresis, **mass spectrometry**, and bioinformatics will be important tools for **protein** and **proteome** anal. in the post-genome era. **Protein identification** from electrophoretic gels by **mass spectrometric peptide** mapping or **peptide** sequencing combined with sequence database searching is established and has been applied to numerous biol. systems. We describe current strategies and selected applications in mol. and cell biol. The next challenges are detailed structure/function analyses, which include studying the mol. compn. of **multiprotein** complexes and characterization of secondary modifications of **proteins**. The advantages and limitations of a no. of **mass spectrometry** -based strategies designed for microcharacterization of low amts. of **protein** from electrophoretic gels are discussed and illustrated by examples.
REFERENCE COUNT: 79
REFERENCE(S): (1) Alberts, B; Cell 1998, V92, P291 HCAPLUS
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ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 3 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:704582 HCAPLUS
DOCUMENT NUMBER: 130:64992
TITLE: **Identification** of apoptosis-associated proteins in a human Burkitt lymphoma cell line. Cleavage of heterogeneous nuclear ribonucleoprotein A1 by caspase 3
AUTHOR(S): Brockstedt, Ekkehard; Rickers, Anke; Kostka, Susanne; Laubersheimer, Andreas; Dorken, Bernd; Wittmann-Liebold, Brigitte; Bommert, Kurt; Otto, Albrecht
CORPORATE SOURCE: Proteinchemie Max-Delbruck-Centrum fur Molekulare Medizin Humboldt University of Berlin, Robert Rossle Klinik, Berlin, D-13125, Germany
SOURCE: J. Biol. Chem. (1998), 273(43), 28057-28064
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Apoptosis or programmed cell death is essential in the process of controlling lymphocyte growth and selection. We **identified** **proteins** that are involved in anti-IgM antibody-mediated apoptosis

using a subclone of the human Burkitt lymphoma cell line BL60. Apoptosis-assocd. **proteins** were detected by high resoln. two-dimensional gel electrophoresis on a micropreparative scale. Comparison of the high resoln. two-dimensional gel electrophoresis **protein** patterns from apoptotic and non-apoptotic cells showed differences in .apprx.80 spots including **protein** modifications. Anal. of the predominantly altered **proteins** was performed by internal Edman microsequencing and/or by **peptide mass** fingerprinting using matrix-assisted laser desorption/ionization **mass spectrometry**. Anal. was significantly improved by using new micropreparative high resoln. two-dimensional gels employing high **protein** concns. The following 12 apoptosis-assocd. **proteins** were **identified**: heterogeneous nuclear **ribonucleoprotein** (hnRNP) A1, hnRNP C1/C2, FUSE-binding **protein**, dUTPase, lymphocyte-specific **protein** LSP1, UV excision repair **protein** RAD23 homolog B (HHR23B), 60 S acidic ribosomal **protein** P0 (L10E), heterochromatin **protein** 1 homolog .alpha. (HP1.alpha.), nucleolin, lamin, neutral calponin, and actin. Fragmentation of actin, hnRNP A1, hnRNP C1/C2, 60 S acidic ribosomal **protein** P0, lamin, and nucleolin could be inhibited by benzyloxycarbonyl-Asp(OMe)-Glu(OMe)-Val-Asp(OMe)-fluoromethyl ketone, a selective irreversible inhibitor of CPP32 (caspase 3).

REFERENCE COUNT: 44
REFERENCE(S):
(2) Bazar, L; Oncogene 1995, V10, P2229 HCAPLUS
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(6) Dudley, B; J Biol Chem 1992, V267, P11964 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 4 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:697567 HCAPLUS
DOCUMENT NUMBER: 130:63133
TITLE: Microfabricated device coupled with an electrospray ionization quadrupole time-of- flight **mass spectrometer: protein identifications** based on enhanced-resolution **mass spectrometry** and tandem **mass spectrometry** data
AUTHOR(S): Figeys, Daniel; Lock, Chris; Taylor, Lorne; Aebersold, Ruedi
CORPORATE SOURCE: Institute for Marine Biosciences, National Research Council Canada, Halifax, NS, Can.
SOURCE: Rapid Commun. Mass Spectrom. (1998), 12(20), 1435-1444
CODEN: RCMSEF; ISSN: 0951-4198
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We describe the coupling of a microfabricated fluidic device to an electrospray ionization (ESI) quadrupole time-of-flight **mass spectrometer** (QqTOFMS) for the **identification** of **protein** samples. The microfabricated devices consisted of three reservoirs connected via channels to a main capillary, which in turn was linked via a microspray interface to the QqTOFMS. Here we present

preliminary results obtained using this system. Standardized solns. of myoglobin tryptic digest were analyzed indicating a limit of detection at the low to sub fmol/plL. The combination of the microfabricated device for rapid sample delivery and the rapid acquisition capability, enhanced resoln. and mass accuracy of the QqTOF offers unique possibilities for the rapid **identification** of **proteins** by database searching. This platform can generate MS data suitable for **protein** database searching by the **peptide-mass** fingerprinting approach and MS/MS data suitable for **protein** database searching. Here the results of the two database-searching approaches are compared and the possibilities of combining the two approaches for rapid **identification** of **protein** are discussed. Also, we present a comparison of the results obtained using the three-position microfabricated device coupled to the ESI-QqTOFMS and to an ESI-ion trap MS. Finally the combination of C-terminal 180 labeling of **peptides** and the microfabricated system for automated combined **peptide-mass** fingerprinting and sequence-tag database searching is discussed.

REFERENCE COUNT: 42
REFERENCE(S):
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(9) Figeys, D; Anal Chem 1996, V68, P1822 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 5 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:686618 HCAPLUS
DOCUMENT NUMBER: 130:49374
TITLE: Characterization of Serine and Threonine Phosphorylation Sites in .beta.-Elimination/Ethanethiol Addition-Modified **Proteins** by Electrospray Tandem **Mass Spectrometry** and Database Searching
AUTHOR(S): Jaffe, Howard; Veeranna; Pant, Harish C.
CORPORATE SOURCE: LNC-NINDS Protein/Peptide Sequencing Facility National Institute of Neurological Disorders and Stroke, National Institutes of Health, Bethesda, MD, 20892, USA
SOURCE: Biochemistry (1998), 37(46), 16211-16224
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A new method for the characterization of serine and threonine phosphorylation sites in **proteins** has been developed. After modification of a **phosphoprotein** by .beta.-elimination/ethanethiol addn. and conversion of phosphoserine and phosphothreonine residues to S-ethylcysteinyl or .beta.-methyl-S-ethylcysteinyl residues, the modified **protein** was subjected to proteolytic digestion. Resulting digests were analyzed by a combination of microbore liq. chromatog., electrospray ionization tandem (MS/MS) ion

trap **mass spectrometry** and database searching to **identify** original phosphorylated residues. The computer program utilized (SEQUEST) is capable of **identifying peptides** and modified residues from uninterpreted MS/MS spectra, and using this method, all of the five known phosphorylation sites in bovine .beta.-casein were **identified**. Application of the method to multiply phosphorylated human high mol. wt. neurofilament **protein** (NF-H) resulted in the **identification** of 21 **peptides** and their modified residues and hence, the in vivo phosphorylation sites. These included 26 KSP and 1 KTP site, all of which occur in the KSP repeat C-terminal tail domain (residues 502-823). One site at residue 518 was previously uncharacterized. A novel non-KSP serine at residue 421 near the KLLEGEE region in a IPFSLPE motif was characterized as phosphorylated (or glycosylated). The 27 characterized phosphorylation sites occur at S/TP residues in the following motifs: KSPVKEE, KSPAEAK, KSPEKEE, KSPAEVK, KSPEKAK, KSPPEAK, KSPVKAE, and KTPAKEE. On the basis of kinase consensus sequences, all of these motifs, including the previously unreported KTPAKEE motif, can be phosphorylated by proline-directed kinases. Advantages of the new method vis-a-vis our previously reported method [Jaffe, H., Veeranna, Shetty, K. T., and Pant, H. C. (1998) Biochem. 37, 3931-3940] include (i) prodn. of diastereomers eluting at different retention times increased the chances of **peptide identification**, (ii) increased hydrophobicity and hence retention time of the modified **peptides**, (iii) facilitation of pos. ion prodn., and (i.v.) increased susceptibility to tryptic digestion as a result of conversion of neg. charged phosphorylated residues to neutral S-ethylcysteine or .beta.-methyl-S-ethylcysteine residues.

REFERENCE COUNT: 43
REFERENCE(S):
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(9) Chin, S; J Neurosci 1990, V10, P3714 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L35 ANSWER 6 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:635863 HCAPLUS
DOCUMENT NUMBER: 129:341417
TITLE: Towards an automated approach for **protein identification** in proteome projects
AUTHOR(S): Traini, Mathew; Gooley, Andrew A.; Ou, Keli; Wilkins, Marc R.; Tonella, Luisa; Sanchez, Jean-Charles; Hochstrasser, Denis F.; Williams, Keith L.
CORPORATE SOURCE: Center Analytical Biotechnology, School Biological Sciences, Macquarie University, Sydney, 2109, Australia
SOURCE: Electrophoresis (1998), 19(11), 1941-1949
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The development of automated, high throughput technologies for the rapid **identification** of **proteins** is essential for large-scale **proteome** projects. While a degree of automation already exists in

some stages of the **protein identification** process, such as automated acquisition of matrix assisted laser desorption ionization-time of flight (MALDI-TOF) **mass spectra**, efficient interfaces between different stages are still lacking. The authors report the development of a highly automated, integrated system for large scale **identification** of **proteins** sepd. by 2-D gel electrophoresis, based on **peptide mass** fingerprinting. A prototype robotic system was used to image and excise 288 **protein** spots from an amido black stained polyvinylidene difluoride (PVDF) blot. **Protein** samples were enzymically digested with a com. automated liq. handling system. MALDI-TOF **mass spectrometry** was used to acquire **mass spectra** automatically, and the data analyzed with novel automated **peptide mass** fingerprinting database interrogation software. Using this highly automated system, the authors were able to **identify** 95 **proteins** on the basis of **peptide mass** fingerprinting, isoelec. point and mol. wt., in a period of less than 10 working days. Advantages, problems, and future developments in robotic excision systems, liq. handling, and automated database interrogation software are discussed.

L35 ANSWER 7 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:635861 HCAPLUS
DOCUMENT NUMBER: 129:341416
TITLE: **Identification** of yeast proteins from two-dimensional gels. Working out spot cross-contamination
AUTHOR(S): Parker, Kenneth C.; Garrels, James I.; Hines, Wade; Butler, Erin M.; McKee, Andrew H. Z.; Patterson, Dale; Martin, Steve
CORPORATE SOURCE: PerSeptive Biosystems, Framingham, MA, 01701, USA
SOURCE: Electrophoresis (1998), 19(11), 1920-1932
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB With the complete sequence of the yeast genome now available, efforts by many labs. are underway to **identify** each of the spots on 2-D gels corresponding to the most abundant yeast **proteins**. The high mass accuracy now attainable using matrix assisted laser desorption/ionization (MALDI)-**mass spectrometry** equipped with delayed extn. simplifies the process of **identification**, such that many spots can be unambiguously **identified** in a short period of time merely by **peptide mass** fingerprinting and generally available database matching programs. Although it is not always possible to match spots between gels run by different labs., **proteins** generally yield the same abundant proteolytic fragments when tryptic digestions are performed. Databases contg. these signature **peptides** not only simplify the task of reidentifying **proteins** from different gels, but also make it possible to **identify** small amts. of cross-contaminating **proteins** from different spots, as well as common extraneous contaminants such as human keratins. The authors present data on the **identification** of >20 previously unreported yeast **proteins**

from 2-D gels. Some novel **proteins** were **identified** from randomly analyzed spots. Focusing on 14 spots in a narrow-pH-range gel, the authors demonstrate how organizing peak-table data and **peptide** match-list data into databases enables the **identification** of a larger % of the peaks.

L35 ANSWER 8 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:386801 HCAPLUS
DOCUMENT NUMBER: 129:51685
TITLE: Two-dimensional electrophoresis of human placental mitochondria and **protein identification** by **mass spectrometry**. Toward a human mitochondrial **proteome**
AUTHOR(S): Rabilloud, Thierry; Kieffer, Sylvie; Procaccio, Vencent; Louwagie, Mathilde; Courchesne, Paul L.; Patterson, Scott D.; Martinez, Pascal; Garin, Jerome; Lunardi, Joel
CORPORATE SOURCE: CEA-Lab. BioEnergetique Cellulaire Pathologique, Grenoble, F-38054, Fr.
SOURCE: Electrophoresis (1998), 19(6), 1006-1014
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Owing to the complexity of higher eukaryotic cells, characterization of a complete proteome is likely to be difficult to achieve. Advantage can be taken of the cell compartmentalization to build organelle proteomes, which can moreover be viewed as specialized tools to study specifically the biol. and "physiol." of the target organelle. Within this frame, the authors report here the construction of the human mitochondrial proteome, using placenta as the source tissue. **Protein identification** was carried out mainly by **peptide mass** fingerprinting, but other methods were also used (N-terminal microsequencing, blotting). The optimization steps in 2-dimensional (2-D) electrophoresis needed for proteome research are discussed. The relative paucity of data concerning mitochondrial proteins is still the major limiting factor in building the corresponding proteome, which should be a useful tool for researchers working on human mitochondria and their deficiencies.

L35 ANSWER 9 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:386799 HCAPLUS
DOCUMENT NUMBER: 129:105694
TITLE: The **identification** of peptide modifications derived from gel-separated proteins using electrospray triple quadrupole and ion trap analyses
AUTHOR(S): Swiderek, Kristine M.; Davis, Michael T.; Lee, Terry D.
CORPORATE SOURCE: Beckman Research Inst., City Hope, Duarte, CA, USA
SOURCE: Electrophoresis (1998), 19(6), 989-997
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Microspray tandem **mass spectrometry** (MS/MS) in combination with database search routines has become a powerful tool for the **identification** of **proteins** from femtomole amts. of material following gel electrophoresis and in-gel digestion procedures. Artifactual modification of susceptible residues can arise during gel electrophoresis, leading to unexpected **peptide mass** shifts during mass anal. Collision-induced dissocn. (CID) spectra generated from these derivatized **peptides** can defy direct interpretation by automated database search routines and remain unidentified. The authors evaluate the MS/MS spectra of **peptides** carrying oxidized derivs. of Trp and Met residues, and various modifications of Cys. The authors demonstrate that certain of these modifications generate characteristic fragmentation patterns or "fingerprints", during CID anal., the knowledge of which can facilitate the interpretation of the spectra. The authors show that these signature fragment ions are predominantly produced during the CID anal. of singly charged ions although they can be obsd. in the MS/MS spectra of the doubly charged species as well. In other cases, the CID spectrum lacks a characteristic fingerprint and the modification remains silent. CID spectra of related **peptides**, differing only by their modifications, are similar and all or part of the fragment ion spectra will have shifted by a discreet mass, which facilitates the **identification** of the modified residue. At the same time, the comparison of related spectra can prevent misinterpretations such as the assignment of a residue mass to the wrong **amino** acid or a neutral loss fragment ion to a y- or b-ion.

L35 ANSWER 10 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:386797 HCAPLUS
DOCUMENT NUMBER: 129:51121
TITLE: Rapid **identification** of comigrating gel-isolated **proteins** by ion trap-**mass spectrometry**
AUTHOR(S): Arnott, David; Henzel, William J.; Stults, John T.
CORPORATE SOURCE: Protein Chem. Dep., Genentech Inc., San Francisco, CA, 94080, USA
SOURCE: Electrophoresis (1998), 19(6), 968-980
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In the search for novel nuclear binding **proteins**, 2 bands from a Na dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) gel were analyzed and each was found to contain a no. of **proteins** that subsequently were **identified** by tandem **mass spectrometry** (MS/MS) on a quadrupole ion trap instrument. The bands were digested with trypsin in situ on a polyvinylidene difluoride (PVDF) membrane following electroblot transfer. Anal. of a 2.5% aliquot of each **peptide** mixt. by matrix assisted laser desorption/ ionization-**mass spectrometry** (MALDI-MS) followed by an initial database search with the **peptide** masses failed to **identify** the **proteins**. The **peptides** were sepd. by reversed-phase capillary HPLC in anticipation of subsequent Edman

degrdn., but mass anal. of the chromatog. fractions by MALDI-MS revealed multiple, coeluting **peptides** that precluded this approach. Selected fractions were analyzed by capillary HPLC-electrospray ionization-ion trap **mass spectrometry**. Tandem **mass spectrometry** provided significant fragmentation from which full or partial sequence was deduced for a no. of **peptides**. 2 Stages of fragmentation by multistage **mass spectrometry** were used in a case to det. addnl. sequence. Database searches, each using a single **peptide mass** plus partial sequence, **identified** 4 **proteins** from a single electrophoretic band at 45 kDa, and 4 **proteins** from a 2nd band at 60 kDa. Many of these **proteins** were derived from human keratin. The **protein identifications** were corroborated by the presence of multiple matching **peptide** masses in the MALDI-MS spectra. A novel sequence, not found in **protein** or DNA databases, was detd. by interpretation of the MS/MS data. These results demonstrate the power of the quadrupole ion trap for the **identification** of multiple **proteins** in a mixt., and for de novo detn. of **peptide** sequence. Reanal. of the fragmentation data with a modified database searching algorithm showed that the same sets of **proteins** were **identified** from a limited no. of fragment ion masses, in the absence of **mass spectral** interpretation or **amino** acid sequence. The implications for **protein identification** solely from fragment ion masses are discussed, including advantages for low signal levels, for a redn. of the necessary interpretation expertise, and for increased speed.

L35 ANSWER 11 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:386796 HCAPLUS
DOCUMENT NUMBER: 129:51120
TITLE: Optimization of capillary chromatography ion trap-**mass spectrometry** for **identification** of gel-separated **proteins**
AUTHOR(S): Courchesne, Paul L.; Jones, Michael D.; Robinson, John H.; Spahr, Chris S.; McCracken, Susan; Bentley, David L.; Luethy, Roland; Patterson, Scott D.
CORPORATE SOURCE: Amgen Center, Amgen Inc., Thousand Oaks, CA, 91320, USA
SOURCE: Electrophoresis (1998), 19(6), 956-967
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The current paradigm for **protein identification** using **mass spectrometric** derived **peptide-mass** and fragment-ion data employs computer algorithms which match uninterpreted or partially interpreted fragment-ion data to sequence databases, both **protein** and translated nucleotide sequence databases. Nucleotide sequence databases continue to grow at a rapid rate for some species, providing an unsurpassed resource for **protein identification** in those species. Ion-trap **mass spectrometers** with their ability to rapidly generate fragment-ion spectra in a data-dependent manner with high sensitivity and accuracy has

led to their increased use for **protein identification**. The authors have investigated various parameters on a com. ion trap-**mass spectrometer** to enhance the ability to **identify peptides** sepd. by capillary reversed phase-high performance liq. chromatog. (RP-HPLC) coupled online to the **mass spectrometer**. By systematically evaluating the std. parameters (ion injection time and no. of microscans) together with selection of multiple ions from the full mass range, improved tandem **mass spectrometry** (MS/MS) spectra were generated, facilitating **identification** of **proteins** at a low pmol level. Application of this technol. to the **identification** of a std. **protein** and an unknown from an affinity-enriched mixt. are shown.

L35 ANSWER 12 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:386795 HCAPLUS
DOCUMENT NUMBER: 129:51119
TITLE: Capillary column chromatography improves sample preparation for mass spectrometric analysis. Complete characterization of human .alpha.-enolase from tow-dimensional gels following in situ proteolytic digestion
AUTHOR(S): Reid, Gavin E.; Rasmussen, Richele K.; Dorow, Donna S.; Simpson, Richard J.
CORPORATE SOURCE: Joint Protein Structure Lab., Ludwig Inst. Cancer Research, Royal Melbourne Hospital, Parkville, 3050, Australia
SOURCE: Electrophoresis (1998), 19(6), 946-955
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors evaluate capillary column RP-HPLC/**mass spectrometric** approaches for **identifying** and characterizing 2-DE resolved **proteins**. Stable and efficient 0.20 mm and 0.32 mm internal diam. (ID) fused-silica columns with hydrophilic polyvinylidene difluoride (PVDF) frits were fabricated and slurry packed with 7 .mu.m spherical, 300 A pore size, C8 bonded phase silica particles. The authors show that capillary column chromatog. is a rapid and efficient desalting/ concg. (ON/OFF) technique for sample cleanup prior to **protein identification** by **peptide-mass** fingerprinting using matrix-assisted laser desorption ionization (MALDI)-time-of-flight **mass spectrometry**. While marginally more **peptide mass** information can be obtained by stepped elution of the **peptide** mixt. with increasing concns. of org. solvent, best results were obtained by fractionation of the **peptide** mixt. using a linear 60 min gradient. A salient feature was the observation that, in contrast to the stepped elution and gradient approaches, the ionization of **peptide** T1 (m/z 2402.2 SGETEDTFIADLVV(PeCys)TGQIK) was almost completely suppressed using the ON/OFF approach. Maximal **amino** acid sequence coverage, a necessary prerequisite for complete characterization of a **protein**, was accomplished using a capillary column (0.2 mm ID) directly coupled with an electrospray ionization (ESI) ion-trap tandem **mass spectrometer**.

For example, from an in situ tryptic digest of .alpha.-enolase isolated by 2-DE from the human breast carcinoma cell line MDA-MB231, 71% of the **amino** acid sequence was obtained. In addn. to **identifying** 2 possible N-terminal acetylated .alpha.-enolase variants, Asn153Asp and Ile152Asp/Asn153Ile, the tandem **mass spectrometric** data revealed the presence of a no. of process-induced modifications of .alpha.-enolase such as Met oxidn. and Cys amidoethylation.

L35 ANSWER 13 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:386789 HCAPLUS
DOCUMENT NUMBER: 129:14031
TITLE: Database searching using mass spectrometry data
AUTHOR(S): Yates, John R., III
CORPORATE SOURCE: Dep. Molecular Biotechnol., Univ. Washington, Seattle, WA, 98185, USA
SOURCE: Electrophoresis (1998), 19(6), 893-900
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 48 refs. Large-scale DNA sequencing is creating a sequence infrastructure of great benefit to **protein** biochem. Concurrent with the application of large-scale DNA sequencing to whole genome anal., **mass spectrometry** has attained the capability to rapidly, and with remarkable sensitivity, det. wts. and **amino** acid sequences of **peptides**. Computer algorithms were developed to use the 2 different types of data generated by **mass spectrometers** to search sequence databases. When a **protein** is digested with a site-specific protease, the mol. wts. of the resulting collection of **peptides**, the mass map or fingerprint, can be detd. using **mass spectrometry**. The mol. wts. of the set of **peptides** derived from the digestion of a **protein** can then be used to **identify** the **protein**. Several different approaches were developed. **Protein identification** using **peptide mass** mapping is an effective technique when studying organisms with completed genomes. A 2nd method is based on the use of data created by tandem **mass spectrometers**. Tandem **mass spectra** contain highly specific information in the fragmentation pattern as well as sequence information. This information was used to search databases of translated **protein** sequences as well as nucleotide databases such as expressed sequence tag (EST) sequences. The ability to search nucleotide databases is an advantage when analyzing data obtained from organisms whose genomes are not yet completed, but a large amt. of expressed gene sequence is available (e.g., human and mouse). Furthermore, a strength of using tandem **mass spectra** to search databases is the ability to **identify proteins** present in fairly complex mixts.

L35 ANSWER 14 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:350386 HCAPLUS
DOCUMENT NUMBER: 129:78616
TITLE: **Mass spectrometry** of **peptides** in neuroscience

AUTHOR(S): Nilsson, Carol L.; Karlsson, Gosta; Bergquist, Jonas; Westman, Ann; Ekman, Rolf
CORPORATE SOURCE: Institute of Clinical Neuroscience, Department of Psychiatry and Neurochemistry, Sahlgrenska University Hospital/Molndal, Goteborg University, Moelndal, S-431, Swed.
SOURCE: Peptides (N. Y.) (1998), 19(4), 781-789
CODEN: PPTDD5; ISSN: 0196-9781
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 53 refs. focuses on the contributions of modern **mass spectrometry** to **neuropeptide** research. An introduction to newer **mass spectrometric** techniques is provided. Also, the use of **mass spectrometry** in combination with high-resoln. sepn. techniques for **neuropeptide identification** in biol. samples is illustrated. The **amino** acid sequence information that is important for the **identification** and anal. of known, novel, or chem. modified **neuropeptides** may be obtained using **mass spectrometric** techniques. Because **mass spectrometry** techniques can be used to reflect the dynamic properties assocd. with **neuropeptide** processing in biol. systems, they may be used in the future to monitor **peptide** profiles within organisms in response to environmental challenges such as disease and stress.

L35 ANSWER 15 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1998:75036 HCAPLUS
DOCUMENT NUMBER: 128:189941
TITLE: **Mass spectrometry** and the age of the **proteome**
AUTHOR(S): Yates, John R., III
CORPORATE SOURCE: Department of Molecular Biotechnology, School of Medicine, University of Washington, Seattle, WA, 98195-7730, USA
SOURCE: J. Mass Spectrom. (1998), 33(1), 1-19
CODEN: JMSPFJ; ISSN: 1076-5174
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 136 refs. **Mass spectrometry** has become an important technique to correlate **proteins** to their genes. This has been achieved, in part, by improvements in ionization and mass anal. techniques concurrently with large-scale DNA sequencing of whole genomes. Genome sequence information has provided a convenient and powerful resource for **protein identification** using data produced by matrix-assisted laser desorption/ionization time-of-flight (MALDI/TOF) and tandem **mass spectrometers** . Both of these approaches have been applied to the **identification** of electrophoretically sepd. **protein** mixts. New methods for the direct **identification** of **proteins** in mixts. using a combination of enzymic proteolysis, liq. chromatog. sepn., tandem **mass spectrometry** and computer algorithms which match **peptide** tandem **mass**

spectra to sequences in the database are also emerging. This tutorial review describes the principles of ionization and mass anal. for **peptide** and **protein** anal. and then focuses on current methods employing MALDI and electrospray ionization for **protein identification** and sequencing. Database searching approaches to **identify proteins** using data produced by MALDI/TOF and tandem **mass spectrometry** are also discussed.

L35 ANSWER 16 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:797221 HCAPLUS
DOCUMENT NUMBER: 128:112425
TITLE: **Protein identification** from 2-DE gels by MALDI **mass spectrometry**
AUTHOR(S): Jungblut, Peter; Thiede, Bernd
CORPORATE SOURCE: Proteinanalysis, Max-Planck-Institute for Infectionbiology, Berlin, D-10117, Germany
SOURCE: Mass Spectrom. Rev. (1997), 16(3), 145-162
CODEN: MSRVD3; ISSN: 0277-7037
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 149 refs. Two-dimensional electrophoresis (2-DE) allows the sepn. of **proteins** at the level of **protein** species, which are defined by their chem. structure. Each chem. modification leads to a new **protein** species. Prerequisites for investigations of **protein** species are reproducible sample prepn., large gels (20 .times. 30 cm and larger), high sensitive detection methods, automated evaluation of gels, and sensitive methods for **identification** of 2-DE-sepd. **protein** species. MALDI **mass spectrometry** with its sensitivity in the fmol range fits with the sensitivity of **protein** detection on 2-De gels. **Protein mass** detn., **peptide mass** mapping, post-source decay sequencing, and ladder sequencing by MALDI-MS in combination with genome databases have the potential for complete structural investigation on the **protein** species level. The discrimination of 19 cryst. species of mouse eye lens and of 54 human heart heat-shock **protein** 27 species shows the capacity of the combination of 2-DE with MALDI-MS.

L35 ANSWER 17 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:741808 HCAPLUS
DOCUMENT NUMBER: 128:84831
TITLE: Development of carboxyl-terminal sequencing methods for **proteins** and **peptide** by the use of FAB **mass spectrometry** and perfluoric acid
AUTHOR(S): Tsugita, Akira
CORPORATE SOURCE: Research Institute for Biosciences, Science University of Tokyo, Noda, 278, Japan
SOURCE: J. Mass Spectrom. Soc. Jpn. (1997), 45(5), 561-589
CODEN: JMSJEY; ISSN: 1340-8097
PUBLISHER: Nippon Shitsuryo Bunseki Gakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB We have developed the following unique methods essentially for carboxyl

(C)-terminal sequencing of proteins and peptides. The first and important observation was the successive truncation reaction of peptide with the use of 90% pentafluoropropionic acid (PFPA) and heptafluorobutyric acid (HFBA) at 90.degree.C for 4-24 h by FAB and ESI-MS. This observation indicated two informations, one of which was the reaction-intermediate to be the prediction of the oxazolones at resp. carboxyl termini of the truncated fragments, and the other was internal bond specific cleavages of carboxyl side of aspartic acid residue (Asp-C) and amino side of serine residue (Ser-N) as the side-reactions. The formation of oxazolone promoted using perfluorate anhydride. The extensive successive truncation was also carried out even at -20.degree.C within 1 h by the use of the perfluorate anhydride in acetonitrile soln. The side reactions, Asp-C and Ser-N were further studied; 0.2% PFPA aq. vapor at 60.degree.C for 24 h selectively cleaved ASp-Pro bond (60.degree.C, h) and the same acid vapor at 90.degree.C for 4-8 h cleaved Asp-C. An aq. 90% PFPA vapor at 25.degree.C for 48 h made N-O peptidyl shift at Ser/Thr. This was reacted with a vapor of 20% acetic anhydride and 1% acetic acid in acetoritrile at 60.degree.C for 1 h. The reaction acetylated the free NH2-groups of the Ser/Thr and the shifted peptide fragments. And finally 20% pimethylaminoethanol (DMAE) aq. soln. at 60.degree.C for 30 min cleaved the O-ester peptide fragment off from OH-group of Ser/Thr residue. These two specific cleavages can be used for **protein-identification** by the aid of "**peptide mass** databases" made from protein sequence database. The successive truncation accompanied by Asp-C or Ser-N cleavages with 90% PFPA at 90.degree.C for 1, 2,4, and 8 h yielded multi-C-terminal sequences of protein. The data of several residues at several sites in protein provided information for **protein identification** again as well for general gene technol. In the last two methodologies TOF-MS and FAB-MS were efficiently employed. A step wise C-terminal sequence method has been developed from the successive truncation reactions, which composed of the following three reactions: (1) formation of oxazolone and acetylation of the N-terminus with a vapor of acetic anhydride with 10% acetic acid at 60.degree.C for 1 h; (2) cleavage off the C-terminal amino acid from the oxazolone and esterification of the peptide, and liberation of the C-terminal amino acid with a vapor of 5% PFPA in methanol (ethanol) soln. at 5.degree.C for 5 min; and (3) hydrolysis of the peptide ester with 20% DMAE aq. solns. at 60.degree.C for 10 min. And the products are ready to the next step reaction.

L35 ANSWER 18 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER:	1997:702370 HCAPLUS
DOCUMENT NUMBER:	128:32037
TITLE:	**Identification** of the Components of Simple Protein Mixtures by High-Accuracy **Peptide Mass** Mapping and Database Searching
AUTHOR(S):	Jensen, Ole N.; Podtelejnikov, Alexandre V.; Mann, Matthias
CORPORATE SOURCE:	Protein Peptide Group, European Molecular Biology Laboratory (EMBL), Heidelberg, D-69117, Germany
SOURCE:	Anal. Chem. (1997), 69(23), 4741-4750 CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER:	American Chemical Society
DOCUMENT TYPE:	Journal

LANGUAGE: English
AB **Peptide mass** mapping by matrix-assisted laser desorption/ionization (MALDI) followed by database searching with the set of measured **peptide** masses is now a powerful method for the **identification** of pure **proteins**. **Protein** mixts.-such as frequently occur due to comigration in polyacrylamide gel bands-have hitherto required **protein** sequencing. Here we demonstrate that such **protein** bands can also be analyzed by **peptide mass** mapping alone. Database searching with the complete list of **peptide** masses detd. by delayed-extn. MALDI **mass spectrometry** with a mass error of less than 30 ppm retrieves the most prominent **protein** in a mixt. In a second step, the **protein identity** is further confirmed by matching as many of the measured **peptide** masses as possible to the retrieved **amino** acid sequence. **Peptide** masses remaining after this "pass search" are searched again to **identify** the next component in the **protein** mixt. This iterative process is repeated until all major ion signals are accounted for. **Protein** mixts. consisting of two or more individual components in a single gel band can be analyzed, further increasing the general applicability of MALDI **peptide** mapping for **protein identification**.

L35 ANSWER 19 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:674722 HCAPLUS
DOCUMENT NUMBER: 127:343409
TITLE: Emerging tandem **mass spectrometry** techniques for the rapid **identification** of **proteins**
AUTHOR(S): Dongre, Ashok R.; Eng, Jimmy K.; Yates, John R., III
CORPORATE SOURCE: Department of Molecular Biotechnology, University of Washington, Seattle, WA, 98195, USA
SOURCE: Trends Biotechnol. (1997), 15(10), 418-425
CODEN: TRBIDM; ISSN: 0167-7799
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 68 refs. State-of-the-art techniques such as liq.-chromatog./electrospray-ionization tandem **mass spectrometry** have, in conjunction with database-searching computer algorithms, revolutionized the anal. of biochem. species from complex biol. mixts. With these techniques, it is now possible to perform high-throughput **protein identification** at picomolar-to-subpicomolar levels from **protein** mixts. This article provides an overview of the techniques and methodols. available for the structural elucidation and **identification** of **proteins** and **peptides** from complex biol. samples.

L35 ANSWER 20 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:462934 HCAPLUS
DOCUMENT NUMBER: 127:187662
TITLE: Novel techniques for **identification** and characterization of proteins loaded on gels in femtomol amounts

AUTHOR(S): Gevaert, Kris; De Mol, Hans; Verschelde, Jean-Luc; Van Damme, Jozef; De Boeck, Stefaan; Vandekerckhove, Joel
CORPORATE SOURCE: Flanders Interuniversity Institute for Biotechnology, Department of Biochemistry, Faculty of Medicine, Universiteit Gent, Belg.
SOURCE: J. Protein Chem. (1997), 16(5), 335-342
CODEN: JPCHD2; ISSN: 0277-8033
PUBLISHER: Plenum
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A combination of techniques is presented allowing gel-purified **protein identification** in the femtomol range using matrix-assisted-laser-desorption-ionization **mass spectrometry**. The **proteins** are detected in the primary gel by sensitive neg. staining procedure, transferred, and concd. in a secondary gel matrix. There, they are digested in the presence of H2 18O and their sequences are predicted (1) by **peptide mass** fingerprinting, (2) by comparing the post-source-decay (PSD) spectra with theor. spectra of candidate isobaric **peptides** using a computer algorithm called MassFrag, and (3) by a manual readout of the 18O/16O-labeled fragmentation ions in the PSD spectra.

L35 ANSWER 21 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:336646 HCAPLUS
DOCUMENT NUMBER: 127:62749
TITLE: A two-dimensional gel database of human colon carcinoma proteins
AUTHOR(S): Ji, Hong; Reid, Gavin E.; Moritz, Robert L.; Eddes, James S.; Burgess, Antony W.; Simpson, Richard J.
CORPORATE SOURCE: Joint Protein Structure Laboratory, Ludwig Institute Cancer Research (Melbourne Branch) and Walter and Eliza Hall Medical Research, Parkville, Australia
SOURCE: Electrophoresis (1997), 18(3-4), 605-613
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The master two-dimensional gel database of human colon carcinoma cells currently lists cellular **proteins** from normal crypts and the colorectal cancer cell lines LIM 1863, LIM 1215 and LIM 1899 (Ward et al., 1990; Ji et al., 1994). Updated 2-dimensional electrophoretic (2-DE) maps of cellular **proteins** from LIM 1215 cells acquired under both nonreducing and reducing conditions are presented. Fifteen cellular **proteins** are **identified** in the reducing 2-DE gel map and 7 in the nonreducing gel map, along with a tabular listing of their Mr/pI loci and mode of **identification**. We also include our **mass spectrometry**-based procedures for **identifying** 2-DE-resolved **proteins**. This procedure relies on a combination of capillary column (0.10-0.32 mm internal diam.) reversed-phase HPLC **peptide** mapping of in-gel digested **proteins**, **peptide mass** fingerprinting, sequence anal. by either collision-induced dissocn. or post-source-decay fragmentation, and **protein identification** using available database search algorithms. These data, and descriptions of the

microtechniques employed in this lab. for **identifying** 2-DE resolved **proteins** can be accessed via the Internet URL: http://www.ludwig.edu.au.

L35 ANSWER 22 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:336147 HCAPLUS
DOCUMENT NUMBER: 127:62707
TITLE: Probing **protein** function using a combination of gene knockout and **proteome** analysis by **mass spectrometry**
AUTHOR(S): Dainese, Paola; Staudenmann, Werner; Quadroni, Manfredo; Korostensky, Chantal; Gonnet, Gaston; Kertesz, Michael; James, Peter
CORPORATE SOURCE: Protein Chemistry Laboratory, Swiss Federal Institute Technology, ETH-Zentrum, Zurich, Switz.
SOURCE: Electrophoresis (1997), 18(3-4), 432-442
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Recently the detn. of the genome sequences of three prokaryotes (Haemophilus influenzae, Methanococcus jannaschii and Mycoplasma genitalium) as well as the first eucaryotic genome (Saccharomyces cerevisiae) were completed. Between 40-60% of the genes were found to code for **proteins** to which no function could be assigned. We describe an approach which combines **proteome** anal. (mapping of expressed **proteins** isolated by two-dimensional polyacrylamide gel electrophoresis to the genome) with genetic manipulations to study the complex pattern of **protein** regulation occurring in Escherichia coli in response to sulfate starvation. We have previously described the upregulation of eight spots on two-dimensional (2-D) gels in response to sulfate starvation and the assignment of six of these to entries in the E. coli genome sequence (Quadroni et al., Eur. J. Biochem. 1996, 239, 773-781). Here we describe the **identification** of the remaining two **proteins** which are encoded in a sulfate-controlled operon in the 21.5' region of the E. coli genome. Upregulated **protein** spots were cut from multiple 2-D gels collected and run on a modified funnel gel to conc. the **proteins** and remove the sodium dodecyl sulfate before digestion. The **peptide** masses obtained from the digests were used to search the SwissProt database or a six-frame translation of the EMBL DNA database using a **peptide** **mass** fingerprinting algorithm. A digest can be reanalyzed after deuterium exchange to obtain a second, orthogonal data set to increase the confidence level of **protein** **identification**. The digests of the remaining unidentified **proteins** were used for **peptide** fragment generation using either post-source decay in a matrix-assisted laser desorption ionization (MALDI) time-of-flight **mass spectrometer** or collision-induced dissocn. (CID) coupled **mass spectrometry** (MS/MS) with triple stage quadrupole or ion trap **mass spectrometers**. The spectra were used as **peptide** fragment fingerprints to search the SwissProt and EMBL databases.

L35 ANSWER 23 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1997:335482 HCAPLUS
DOCUMENT NUMBER: 127:62733
TITLE: **Identification** of mouse liver **proteins** on two-dimensional electrophoresis gels by matrix-assisted laser desorption/ionization **mass spectrometry** of in situ enzymic digests
AUTHOR(S): O'Connell, Kathy L.; Stults, John T.
CORPORATE SOURCE: Protein Chemistry Department, Genentech, Inc., South San Francisco, CA, USA
SOURCE: Electrophoresis (1997), 18(3-4), 349-359
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A no. of **proteins** from a silver-stained two-dimensional (2-D) electrophoresis gel of mouse liver whole-cell lysate were **identified** by **peptide mass** mapping and sequence database searching. The excised **protein** spots were processed by in situ redn. and alkylation, followed by Lys-C digestion. The masses of the resulting **peptide** mixts. were measured with a matrix-assisted laser desorption/ionization (MALDI) reflection-time-of-flight **mass spectrometer**. These masses were used successfully to search a **protein** sequence database. Optimized silver staining and digestion protocols allowed **proteins** to be **identified** routinely at the low picomole level. The high mass accuracy and resoln. provided by delayed extn. were important for high specificity in the database search. Fragment ion data obtained by MALDI post-source decay (PSD) measurements not only provided confirmation of **peptide identification**, but could be used to **identify** the **protein** from a single **peptide** without spectral interpretation.

L35 ANSWER 24 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1997:20403 HCAPLUS
DOCUMENT NUMBER: 126:56979
TITLE: **Identification** of proteins of the yeast protein map using genetically manipulated strains and **peptide-mass** fingerprinting
AUTHOR(S): Sagliocco, Francis; Guillemot, Jean-Claude; Monribot, Christelle; Capdevielle, Joel; Perrot, Michel; Ferran, Edgardo; Ferrara, Pascual; Boucherie, Helian
CORPORATE SOURCE: CNRS, Institut de Biochimie et Genetique Cellulaires, Bordeaux, 33077, Fr.
SOURCE: Yeast (1996), 12(15), 1519-1533
CODEN: YESTE3; ISSN: 0749-503X
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In this study we used genetically manipulated strains to **identify** **polypeptide** spots of the **protein** map of Saccharomyces cerevisiae. Thirty-two novel **polypeptide** spots were **identified** using this strategy. They corresponded to the product of 23 different genes. We also explored the possibilities of using

peptide-mass fingerprinting for the **identification** of **proteins** sepd. on our gels. According to this strategy, **proteins** contained in spots are digested with trypsin and the masses of generated **peptides** are detd. by matrix-assisted laser desorption-ionization **mass spectrometry** (MALDI-MS). The **peptide** masses are then used to search a yeast **protein** database for **proteins** that match the exptl. data. Application of this strategy to previously **identified polypeptide** spots gave evidence of the feasibility of this approach. We also report predictions on the **identities** of nine u MALDI-MS.

L35 ANSWER 25 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:746783 HCAPLUS
DOCUMENT NUMBER: 126:101318
TITLE: Linking genome and **proteome** by **mass spectrometry**: large-scale **identification** of yeast **proteins** from two dimensional gels
AUTHOR(S): Shevchenko, Andrej; Jensen, Ole N.; Podtelejnikov, Alexandre V.; Sagliocco, Francis; Wilm, Matthias; Vorm, Ole; Mortensen, Peter; Shevchenko, Anna; Boucherie, Helian; Mann, Matthias
CORPORATE SOURCE: Peptide Protein Group, European Mol. Biol. Lab., Heidelberg, 69012, Germany
SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1996), 93(25), 14440-14445
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The function of many of the uncharacterized open reading frames discovered by genomic sequencing can be detd. at the level of expressed gene products, the **proteome**. However, **identifying** the cognate gene from minute amts. of **protein** has been one of the major problems in mol. biol. Using yeast as an example, we demonstrate here that **mass spectrometric protein identification** is a general soln. to this problem given a completely sequenced genome. As a first screen, our strategy uses automated laser desorption ionization **mass spectrometry** of the **peptide** mixts. produced by in-gel tryptic digestion of a **protein**. Up to 90% of **proteins** are **identified** by searching sequence data bases by lists of **peptide** masses obtained with high accuracy. The remaining **proteins** are **identified** by partially sequencing several **peptides** of the unsepd. mixt. by nanoelectrospray tandem **mass spectrometry** followed by data base searching with multiple **peptide** sequence tags. In blind trials, the method led to unambiguous **identification** in all cases. In the largest individual **protein identification** project to date, a total of 150 gel spots - many of them at subpicomole amts. - were successfully analyzed, greatly enlarging a yeast two-dimensional gel data base. More than 32 **proteins** were novel and matched to previously uncharacterized open reading frames in the yeast genome. This

study establishes that **mass spectrometry** provides the required throughput, the certainty of **identification**, and the general applicability to serve as the method of choice to connect genome and **proteome**.

L35 ANSWER 26 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:659661 HCAPLUS
DOCUMENT NUMBER: 126:31620
TITLE: Search of sequence databases with uninterpreted high-energy collision-induced dissociation spectra of peptides
AUTHOR(S): Yates, John R., III; Eng, Jimmy K.; Clauser, Karl R.; Burlingame, Alma L.
CORPORATE SOURCE: Dep. Mol. Biotechnol., Univ. Washington, Seattle, WA, USA
SOURCE: J. Am. Soc. Mass Spectrom. (1996), 7(11), 1089-1098
CODEN: JAMSEF; ISSN: 1044-0305
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The utility of the SEQUEST computer algorithm was broadened to permit correlation of uninterpreted high-energy collision-induced dissocn. spectra of **peptides** with all sequences in a database. SEQUEST now allows for the addnl. fragment ion types obsd. under high-energy conditions. Spectra were analyzed from **peptides** isolated following trypsin digestion of 13 **proteins**. SEQUEST ranked the correct sequence first for 90% (18/20) of the spectra in searches of the OWL database, without constraint by enzyme cleavage specificity or species of origin. All false-positives were flagged by the scoring system. SEQUEST searches databases for sequences that correspond to the precursor ion mass .+-.0.5 u. Preliminary ranking of the top 500 candidates is done by calcn. of fragment ion masses for each sequence, and comparison to the measured ion masses on the basis of ion series continuity, summed ion intensity, and immonium ion presence. Final ranking is done by construction of model spectra for the 500 candidates and constructing/performing of a cross-correlation anal. with the actual spectrum. Given the need to relate mounting genome sequence information with corresponding suites of **proteins** that comprise the cellular mol. machinery, tandem **mass spectrometry** appears destined to play the leading role in accelerating **protein identification** on the large scale required.

L35 ANSWER 27 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:658446 HCAPLUS
DOCUMENT NUMBER: 126:44592
TITLE: **Protein identification** by solid phase microextraction-capillary zone electrophoresis-microelectrospray-tandem **mass spectrometry**
AUTHOR(S): Figeys, Daniel; Ducret, Axel; Yates, John R., III; Aebersold, Ruedi
CORPORATE SOURCE: Department Molecular Biotechnology, Univ. Washington, Seattle, WA, 98195-7730, USA
SOURCE: Nat. Biotechnol. (1996), 14(11), 1579-1583

CODEN: NABIF9; ISSN: 1087-0156
PUBLISHER: Nature Publishing Co.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We describe an anal. system for the rapid **identification** of **proteins** by correlation of tandem **mass spectra** with **protein** sequence databases. The system consists of an integrated solid-phase microextn./capillary zone electrophoresis **peptide** sepn. device that is connected through a microelectrospray ion source to a tandem **mass spectrometer**. The limits of detection are 660 amol of sample at a concn. limit of <33 amol/.mu.L for **peptide mass** measurement, and <10 fmol of sample, at a concn. limit of <300 amol/.mu.L for **peptide** anal. by collision-induced dissocn. By using this system, we **identified** low-nanogram amts. of yeast **proteins** sepd. by high-resoln. 2-dimensional gel electrophoresis.

L35 ANSWER 28 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:593250 HCAPLUS
DOCUMENT NUMBER: 125:269426
TITLE: The **identification** of electrophoretically separated proteins by **peptide mass** fingerprinting
AUTHOR(S): Cottrell, John S.; Sutton, Chris W.
CORPORATE SOURCE: Finnigan MAT Ltd., Hemel Hempstead/Hertfordshire, UK
SOURCE: Methods Mol. Biol. (Totowa, N. J.) (1996), 61(Protein and Peptide Analysis by Mass Spectrometry), 67-82
CODEN: MMBIED; ISSN: 1064-3745
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review and discussion with 28 refs. about the principles and use of the title method to **identify proteins** for which sequences are already known. In a general approach, a **protein** is digested by a proteolytic enzyme, and the resulting digest is analyzed by **mass spectrometry** with matrix-assisted laser desorption/ionization or electrospray ionization. The mass values then are compared with a database of **peptide mass** values, calcd. by applying the enzyme cleavage rules to the entries in one of the major collections of sequence data. By using a scoring algorithm, the closest match or matches are **identified**. **Mass spectrometric** anal. might take 5-10 min/sample, whereas the search itself takes 2 min at most, and under best conditions, substantially <1 pmol of sample is needed for **mass spectrometric** anal.

L35 ANSWER 29 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:338663 HCAPLUS
DOCUMENT NUMBER: 125:79577
TITLE: Application of combined **mass spectrometry** and partial **amino** acid sequence to the **identification** of gel-separated **proteins**
AUTHOR(S): Patterson, Scott D.; Thomas, Didier; Bradshaw, Ralph A.
CORPORATE SOURCE: Amgen Inc., Thousand Oaks, CA, USA

SOURCE: Electrophoresis (1996), 17(5), 877-891
CODEN: ELCTDN; ISSN: 0173-0835
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The combined use of **peptide mass** information with **amino** acid sequence information derived by chem. sequencing or **mass spectrometry** (MS)-based approaches provides a powerful means of **protein identification**. We have used a two-part strategy to **identify proteins** from nerve growth factor (NGF)-stimulated rat adrenal pheochromocytoma cell line PC-12 cell lysates that assoc. with the adaptor **protein** Shc (Shc homologous and collagen **protein**). Initial expts. with metabolically radiolabeled cell exts. sepd. by SDS-PAGE revealed a no. of **proteins** that coimmunopptd. with anti-Shc antibody compared with control (unstimulated) cell exts. The expt. was scaled up and cell lysate from NGF-stimulated PC-12 cells was applied to a glutathione-S-transferase (GST)-Shc affinity column, eluted, sepd. by SDS-PAGE and blotted to Immobilon-CD. The blotted **proteins** were proteolytically digested in situ, and the masses obtained from the extd. **peptides** were used in a **peptide-mass** search program in an attempt to **identify** the **protein**. Even if a strong candidate was found using this search, an addnl. step was preformed to confirm, the **identification**. The mixts. were fractionated by reversed-phase high-performance liq. chromatog. (RP-HPLC) and subjected to chem. sequencing to obtain (partial) sequence information, or post-source decay (PSD-) matrix-assisted laser-desorption ionization (MALDI)-MS to obtain sequence-specific fragment ions. This data was used in a **peptide**-sequence tag search to confirm the **identity** of the **proteins**. This combined approach allowed **identification** of four **proteins** of Mr 43000 to 2000000. In one case the **identified protein** clearly did not correspond to the radiolabeled band, but to a **protein** contaminant from the column. The advantages and pitfalls of the approach are discussed.

L35 ANSWER 30 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:260210 HCAPLUS
DOCUMENT NUMBER: 125:4871
TITLE: **Identification** of human myocardial **proteins** separated by two-dimensional electrophoresis with matrix-assisted laser desorption/ionization **mass spectrometry**
AUTHOR(S): Thiede, Bernd; Otto, Albrecht; Zimny-Arndt, Ursula; Mueller, Eva-Christina; Jungblut, Peter
CORPORATE SOURCE: Max-Delbrueck-Centrum Molekulare Medizin, Berlin, Germany
SOURCE: Electrophoresis (1996), 17(3), 588-99
CODEN: ELCTDN; ISSN: 0173-0835
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The authors optimized the measurement by MALDI-MS for the anal. of proteolytic digests of 2-DE-sepd. proteins. The direct anal. of peptide mixts. can be used for rapid and sensitive **protein**

identification. In some cases, more information about the protein can be obtained by sepg. the peptides by micro high-performance liq. chromatog. (HPLC) before employing MALDI-MS anal. More peptides are found than in the mixt., and comparison of HPLC patterns can reveal some differences to be post-translational modifications of proteins, even in the case of **identical peptide mass** fingerprints. Furthermore, carboxy-terminal sequencing by on-target carboxypeptidase P digestion can be used to confirm the obtained result without the need for more material. The search program FRAGFIT was modified and renamed FRAGMOD to include the modifications of methionine and tryptophan oxidn. and alkylation of cysteine by acrylamide into the mass search. By applying this procedure, 15 proteins were **identified**, among them two different putative phosphorylated forms of two proteins, a putative N-terminal blocking group and four dilated cardiomyopathy-assocd. proteins. The resulting approach for the **identification** may be used for large-scale investigations of 2-DE-sepd. proteins.

L35 ANSWER 31 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:236717 HCAPLUS
DOCUMENT NUMBER: 124:337035
TITLE: **Identification** of electroblotted proteins by **peptide mass** searching of a sequence database
AUTHOR(S): Stults, John T.; Henzel, William J.; Wong, Susan C.; Watanabe, Colin
CORPORATE SOURCE: Protein Chemistry Department, Genentech, Inc., South San Francisco, CA, 94080, USA
SOURCE: Mass Spectrom. Biol. Sci. (1996), 151-70. Editor(s): Burlingame, A. L.; Carr, Steven A. Humana: Totowa, N. J.
CODEN: 62PNAY
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The authors have developed a complimentary approach to **protein** sequencing that **identifies protein** by database searching on the basis of **peptide** masses. The **protein** is digested chem. or enzymically. A **mass spectrum** of the resulting **peptide** mixt. provides a **peptide-mass** fingerprint of the **protein**. A computer program performs a theor. digest of each **protein** in the database and attempts to match those mass lists to the measured **peptide mass** fingerprint within the constraints of the search.

L35 ANSWER 32 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:159516 HCAPLUS
DOCUMENT NUMBER: 124:255186
TITLE: Tracing cell signaling pathways using a combination of 2D gel electrophoresis and mass spectrometry
AUTHOR(S): Quadroni, Manfredo; Corti, Chantal; Staudenmann, Werner; Carafoli, Ernesto; James, Peter
CORPORATE SOURCE: Protein Chemistry and Biochemistry III Laboratories, Swiss Federal Institute Technology, Zurich, 8092, Switz.

SOURCE: Methods Protein Struct. Anal., [Proc. Int. Conf.], 10th (1995), Meeting Date 1994, 187-93. Editor(s): Atassi, M. Zouhair; Appella, Ettore. Plenum: New York, N. Y.
CODEN: 62LPAK
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The title topic is discussed with information on **protein identification** by mass mapping, cell signaling by calcium, application of **mass spectrometric** methods to cell signaling, etc.

L35 ANSWER 33 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:105659 HCAPLUS
DOCUMENT NUMBER: 124:197496
TITLE: **Identification** of proteins from two-dimensional electrophoresis gels by **peptide mass** fingerprinting
AUTHOR(S): Arnott, David P.; Henzel, William J.; Stults, John T.
CORPORATE SOURCE: Protein Chem. Dep., Genentech, Inc., San Francisco, CA, 94080, USA
SOURCE: ACS Symp. Ser. (1996), 619(Biochemical and Biotechnological Applications of Electrospray Ionization Mass Spectrometry), 226-43
CODEN: ACSMC8; ISSN: 0097-6156
DOCUMENT TYPE: Journal
LANGUAGE: English
AB As part of a project to **identify** factors involved in congestive heart failure, differences in **protein** expression levels between normal and enlarged (hypertrophic) heart cells were **identified**. In initial expts. two-dimensional gel electrophoresis was used to sep. the **proteins** from normal neonatal rat cardiac myocytes. The **proteins** were electrobotted to a membrane and **identified** by staining. **Proteins** of interest were cleaved into **peptides** with an in situ enzymic digestion method. The masses of the **peptides** were det. dby capillary high performance liq. chromatog. electrospray ionization **mass spectrometry** and, when possible, partial sequences were obtained by subsequent liq. chromatog. tandem **mass spectrometry** (LC-MS/MS) expts. These data were used to search a **protein** sequence database with the program FRAGFIT. The program theor. cleaves each **protein** in the database. By comparison of the exptl.-detd. **peptide** masses and the theor. masses, the program **identifies** the **protein** if it exists in the database. A partial sequence from the LC-MS/MS expt. was used to increase the specificity of the search. With this approach, eight **proteins** present in low picomole quantities on 2-D gels from cardiac myocytes have been **identified**, with 100 fmol or less of each **peptide** component required for the **mass spectral** expts.

L35 ANSWER 34 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1996:60663 HCAPLUS
DOCUMENT NUMBER: 124:140182
TITLE: **Peptide-mass** profiles of

polyvinylidene difluoride-bound **proteins** by matrix-assisted laser desorption/ionization time-of-flight **mass spectrometry** in the presence of nonionic detergents

AUTHOR(S): Gharahdaghi, Farzin; Kirchner, Michele; Fernandez, Joseph; Mische, Sheenah M.

CORPORATE SOURCE: DNA Technol. Cent., Rockefeller Univ. Protein, New York, NY, 10021, USA

SOURCE: Anal. Biochem. (1996), 233(1), 94-9
CODEN: ANBCA2; ISSN: 0003-2697

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Matrix-assisted laser desorption/ionization time-of-flight **mass spectrometry** (MALDI-TOF MS), in conjunction with enzymic digestion of **proteins** and mol. wt. search of **peptide-mass** database is a powerful technique for **peptide/protein identification**. Ideally, **peptide** mixts. should be compatible with both MALDI-TOF and microsequencing. In the lab., enzymic digestion and extn. of **peptides** from polyvinylidene difluoride (PVDF)-bound **proteins** is performed in the presence of nonionic detergents. However, nonionic detergents have been shown to cause signal suppression in MALDI-TOF anal. This study demonstrates that by using a modified matrix soln., **peptide-mass** fingerprinting of PVDF-bound **proteins** by MALDI-TOF can be obtained in the presence of nonionic detergents such as hydrogenated Triton X-100 (RTX-100), octylglucopyranoside, and Tween 20.

L35 ANSWER 35 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1995:719628 HCAPLUS

DOCUMENT NUMBER: 123:107010

TITLE: Matrix-assisted laser-desorption/ionization **mass spectrometric** approaches for the **identification** of gel-separated **proteins** in the 5-50 pmol range

AUTHOR(S): Patterson, Scott D.

CORPORATE SOURCE: Amgen Inc., Thousand Oaks, CA, USA

SOURCE: Electrophoresis (1995), 16(7), 1104-14
CODEN: ELCTDN; ISSN: 0173-0835

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The ability to **identify** and characterize low picomole quantities of gel-sepd. **proteins** has greatly benefited from recent advancements in **mass spectrometric** anal. methods, particularly **peptide-mass** search routines. The authors are investigating the use of matrix-assisted laser desorption/ionization **mass spectrometry** (MALDI-MS) to gain as much mass information as possible from a single gel-sepd. **protein** species. This report details results obtained from one-dimensional SDS-PAGE sepns., under nonreducing conditions, of known quantities of three **proteins**, followed by blotting to Immobilon-CD. Three methods were used to obtain MALDI-MS data from a single blotted **protein** band: (1) direct MALDI-MS of .apprx.10% of the band, (2) CNBr cleavage of another .apprx.10% of the band, and (3) enzymic (**endoproteinase** Lys-C) digestion of the remaining

.apprx.70-80% of the band followed by MALDI-MS. At the level of 50 pmol of **protein** loaded onto the gel, data was obtained from all three approaches. At levels down to 5 pmol of **protein** loaded onto the gel, MALDI-MS data was obtained from the latter two methods, CNBr and Lys-C digestions, but not direct MALDI-MS. Sufficient **peptide** masses were obtained from the 5 pmol loads to **identify** two of the three test **proteins** using four mass search programs. Only limited **peptide mass** data was obtained from fetuin, a sialylated **glycoprotein** with six disulfides and no methionines, but it was **identified**.

L35 ANSWER 36 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:707889 HCAPLUS
DOCUMENT NUMBER: 123:105683
TITLE: Reactivation of phosphorylated actin depolymerizing factor and **identification** of the regulatory site
AUTHOR(S): Agnew, Brian J.; Minamide, Laurie S.; Bamburg, James R.
CORPORATE SOURCE: Dep. Biochem. Mol. Biol., Colorado State Univ., Fort Collins, CO, 80523, USA
SOURCE: J. Biol. Chem. (1995), 270(29), 17582-7
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Actin depolymg. factor (ADF) occurs naturally in two forms, one of which contains a phosphorylated Ser and does not bind G-actin or depolymerize F-actin. Removal of this phosphate in vitro by alk. phosphatase restores full F-actin depolymg. activity. To **identify** the phosphorylation site, [32P]pADF was purified and digested with **endoproteinase** Lys-C. The digest contained only one 32P-labeled **peptide**. Further digestion with **endoproteinase** Asp-N and **mass spectrometric** anal. showed that this **peptide** came from the N terminus of ADF. Alk. phosphatase treatment of one Asp-N **peptide** (**mass** 753) converted it to a **peptide** of mass 673, demonstrating that this **peptide** contains the phosphate group. Tandem **mass spectrometric** sequence anal. of this **peptide** **identified** the phosphorylated Ser as the encoded Ser3 (Ser2 in the processed **protein**). HeLa cells, transfected with either chick wild-type ADF cDNA or a cDNA mutated to code for Ala in place of Ser24 or Thr25, express and phosphorylate the exogenous ADF. Cells also expressed high levels of mutant ADF when Ser3 was deleted or converted to either Ala or Glu. However, none of these mutants was phosphorylated, confirming that Ser3 in the encoded ADF is the single in vivo regulatory site.

L35 ANSWER 37 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1995:482008 HCAPLUS
DOCUMENT NUMBER: 122:209020
TITLE: Recognition of the Carboxy-Terminal Peptide in Cyanogen Bromide Digests of Proteins
AUTHOR(S): Murphy, Constance M.; Fenselau, Catherine
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Maryland Baltimore County, Baltimore, MD, 21228,

USA
SOURCE: Anal. Chem. (1995), 67(9), 1644-5
CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Recognition is based on **mass spectrometric** anal. of the **peptide** products before and after reaction with acidic methanol. **Peptides** generated from internal positions in the **protein** are terminated by homoserine lactone, which undergoes methanolysis to add 32 mass units. The **peptide** contg. the original carboxyl terminus is converted to a Me ester, with a mass increment of 14 Da.

L35 ANSWER 38 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:647335 HCAPLUS
DOCUMENT NUMBER: 121:247335
TITLE: **Protein identification** in DNA databases by **peptide mass** fingerprinting
AUTHOR(S): James, Peter; Quadroni, Manfredo; Carafoli, Ernesto; Gonnet, Gaston
CORPORATE SOURCE: Dep. Biology, Swiss Federal Institute Technology, Zurich, 8092, Switz.
SOURCE: Protein Sci. (1994), 3(8), 1347-50
CODEN: PRCIEI; ISSN: 0961-8368
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Proteins can be **identified** using a set of peptide fragment wts. produced by a specific digestion to search a protein database in which sequences have been replaced by fragment wts. calcd. for various cleavage methods. We present a method using multidimensional searches that greatly increases the confidence level for **identification,** allowing DNA sequence databases to be examd. This method provides a link between 2-dimensional gel electrophoresis protein databases and genome sequencing projects. Moreover, the increased confidence level allows unknown proteins to be matched to expressed sequence tags, potentially eliminating the need to obtain sequence information for cloning. Database searching from a mass profile is offered as a free service by an automatic server at the Swiss Federal Institute of Technol. (ETH), Zurich. For information, send an electronic message to the address cbrg@inf.ethz.ch with the line: help mass search, or help all.

L35 ANSWER 39 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:625756 HCAPLUS
DOCUMENT NUMBER: 121:225756
TITLE: Microbore reversed-phase high-performance liquid chromatographic purification of **peptides** for combined chemical sequencing-laser-desorption **mass spectrometric** analysis
AUTHOR(S): Elicone, Christopher; Lui, Mary; Geromanos, Scott; Erdjument-Bromage, Hediye; Tempst, Paul
CORPORATE SOURCE: Molecular Biology Program and Protein Chemistry Laboratory, Memorial Sloan-Kettering Cancer Center (Box 137), 1275 York Avenue, New York, NY, 10021, USA

SOURCE: J. Chromatogr., A (1994), 676(1), 121-37
CODEN: JCRAEY
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An optimized microbore RP-HPLC system (1.0 mm I.D. columns) for the purifn. of low picomole amts. (<5 pmol) of **peptides** is described. It is comprised of com. available columns, instrument components and parts. These were selected on the basis of a comparative evaluation and to yield the highest resoln. and most efficient peak collection. The sensitivity of this system equals, probably surpasses, that of advanced chem. microsequencing for which 2-4 pmol of **peptide** are minimally required. As an automated sequencer cannot be "online" connected with a micro-preparative HPLC system, fractions must be collected and transferred. With a typical flow of 30 .mu.L, efficient manual collection is possible and fractions (about 20 .mu.L in vol.) can still be handled without unacceptable losses, albeit with great precaution. Furthermore, major difficulties were encountered to efficiently and quant. load low- or sub-picomole amts. of **peptide** mixts. onto the RP-HPLC column for sepn. Discipline and rigorous adherence to sample handling protocols are thus on order when working at those levels of sensitivity. With adequate instrumentation and handling procedures in place, we demonstrate that low picomole amts. of **peptides** can now be routinely prepd. for anal. by combined Edman-chem. sequencing-matrix-assisted laser-desorption **mass spectrometry** (MALDI-MS). The integrated method was applied to covalent structural characterization of minute quantities of a gel-purified **protein** of known biol. function but unknown **identity**. The results allowed unambiguous **identification** and illustrated the power of MALDI-MS-aided interpretation of chem. sequencing data: accurate **peptide** masses were crucial for (i) confirmation of the results, (ii) deconvolution of mixed sequences, (iii) proposal of complete structures on the basis of partial sequences, and (i.v.) confirmation of **protein identification** (obtained by database search with a single, small stretch of **peptide** sequence) by "mass matching" of several more **peptides** with predicted proteolytic fragments.

L35 ANSWER 40 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:574143 HCAPLUS
DOCUMENT NUMBER: 121:174143
TITLE: **Protein identification** by **peptide mass** fingerprinting
AUTHOR(S): Cottrell, John S.
CORPORATE SOURCE: Finnigan MAT Ltd., Hemel Hempstead, UK
SOURCE: Pept. Res. (1994), 7(3), 115-18, 120-4
CODEN: PEREEO; ISSN: 1040-5704
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 22 refs. on **protein identification** by **peptide mass** fingerprinting. This review aims to provide an overview of the technique, compare the different database matching algorithms which have been described in the literature, and discuss the practical and theor. factors which influence **identification** accuracy.

L35 ANSWER 41 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:318644 HCAPLUS
DOCUMENT NUMBER: 120:318644
TITLE: **Identification** of transformation-sensitive **proteins** recorded in human two-dimensional gel **protein** databases by **mass spectrometric peptide** mapping alone and in combination with microsequencing
AUTHOR(S): Rasmussen, Hanne H.; Mertz, Ejvind; Mann, Matthias; Roepstorff, Peter; Celis, Julio E.
CORPORATE SOURCE: Inst. Med. Biochem., Aarhus Univ., Aarhus, Den.
SOURCE: Electrophoresis (Weinheim, Fed. Repub. Ger.) (1994), 15(3-4), 406-16
CODEN: ELCTDN; ISSN: 0173-0835
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A comprehensive human keratinocyte two-dimensional (2-D) gel **protein** database was established to study the expression levels and properties of the thousands of **proteins** that orchestrate various keratinocyte functions both in health and disease, cancer included. A major task in establishing such a database is to **identify** known **proteins** in the 2-D gel patterns as well as to reveal hitherto unknown **proteins**. To date, **protein identification** has been performed by one or a combination of the following methods: (1) comigration with known **proteins**, (2) Western blotting using specific antibodies, (3) microsequencing, and (4) vaccinia virus expression of full length cDNAs. Recently, the systematic **identification** of **proteins** has gained a new dimension with the advent of computer programs for searching **peptide** mol. mass databases with exptl. obtained **peptide mass** maps. Here the authors investigate this approach to **identify proteins** that are highly up- or down-regulated in simian virus SV40 transformed human keratinocytes (K14). **Peptide mass** maps of several **proteins**, including keratins 7, 8, 18, and 19 were obtained either by plasma desorption **mass spectrometry** (PDMS) anal. of HPLC-purified **peptides** or by matrix-assisted laser desorption/ionization **mass spectrometry** (MALDI-MS) of total digests. The results demonstrated that **peptide mass** maps can be used for a rapid and sensitive **protein identification** allowing fast screening of **proteins** recorded in 2-D gel databases. The **mass spectrometric** approach when combined with microsequencing strengthened **identification**, and added the possibility of full characterization of posttranslational modifications and sequence variations.

L35 ANSWER 42 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1994:318643 HCAPLUS
DOCUMENT NUMBER: 120:318643
TITLE: Two-dimensional electrophoretic analysis of **proteins** expressed by normal and cancerous human crypts: application of **mass spectrometry** to **peptide-mass**

fingerprinting

AUTHOR(S): Ji, Hong; Whitehead, Robert H.; Reid, Gavin E.; Moritz, Robert L.; Ward, Larry D.; Simpson, Richard J.

CORPORATE SOURCE: Jt. Protein Struct. Lab., Walter and Eliza Hall Inst. Med. Res., Parkville, Australia

SOURCE: Electrophoresis (Weinheim, Fed. Repub. Ger.) (1994), 15(3-4), 391-405
CODEN: ELCTDN; ISSN: 0173-0835

DOCUMENT TYPE: Journal
LANGUAGE: English

AB **Protein** patterns of normal human colonic crypts, isolated from different regions of the large intestine, and several colorectal cancer cell lines were compared using two-dimensional electrophoresis gels (2-DE). As detected by intrinsic radiolabeling and Coomassie Brilliant Blue staining, the **protein** patterns for normal crypts isolated from the ascending, and descending, regions of the colon and the rectum, were almost (>95%) **identical**. While 75-80% of the **protein** spots from normal crypts and the colorectal cancer cell line (LIM 1863), a cell line that grows as organoids and differentiates spontaneously into crypt-like structures in vitro, can be matched, the relative expression levels of a large no. of **proteins** differ. At least 2 **protein** spots (undetectable in the **protein** pattern from normal cells), **proteins** a (Mr .apprx.18,000, pI 6.7-6.9) and b (Mr .apprx.24,000, pI 5.9-6.0), were detected in the 2-DE gel **protein** pattern in the 3 cells lines LIM 1863, LIM 1215, and LIM 1899. The **identity** of these **proteins** is not yet known and further studies are required before they can be considered as potential colon tumor markers. Approx. 60% of the cellular **proteins** from LIM 1215 cells, a colon carcinoma cell line that exhibits many properties assocd. with columnar cells, can be matched with LIM 1863 cells. The results presented here represent an initial phase in the authors' efforts to develop a comprehensive **protein** database for normal human colon cells and several colorectal cancer cell lines. While the authors' initial **protein identification** relied on microsequencing methodologies, the authors are presently evaluating **peptide-mass** fingerprinting, utilizing capillary reversed-phase HPLC, and electrospray **mass spectrometry**, as a means for rapid **identification** of **proteins** at subpicomole levels. Using this approach, **protein** #3 (Mr .apprx. 66,000, pI 6.2) was **identified** as heat shock **protein** 60 from as few as 7 **peptide** masses when they were screened against the mol. wt. search (MOWSE) **peptide-mass** database.

L35 ANSWER 43 OF 48 HCAPLUS COPYRIGHT 2001 ACS

ACCESSION NUMBER: 1994:3992 HCAPLUS
DOCUMENT NUMBER: 120:3992
TITLE: **Peptide mass** maps: A highly informative approach to **protein identification**

AUTHOR(S): Yates, John R., III; Speicher, Stephen; Griffin, Patrick R.; Hunkapiller, Tim

CORPORATE SOURCE: Sch. Med., Univ. Washington, Seattle, WA, 98195, USA
SOURCE: Anal. Biochem. (1993), 214(2), 397-408

CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A computer searching algorithm has been used to **identify** **protein** sequences in the **Protein** Information Resource (PIR) database with **peptide mass** information (mass map) obtained from proteolytic digests of **proteins** analyzed by microcapillary high-performance liq. chromatog. electrospray ionization **mass spectrometry**. A theor. anal. of the cytochrome c family demonstrates the ability to **identify protein** sequences in the PIR database with a high degree of accuracy using a set of six predicted tryptic **peptide** masses. This method was also applied to exptl. detd. **peptide** masses for a small GTP-binding **protein**, a **protein** from pig uterus, the human sex steroid binding **protein**, and a thermostable DNA polymerase. The results demonstrate that a set of obsd. masses which is less than 50% of the total no. of predicted masses can be used to **identify** a **protein** sequence in the database. For the anal. presented in this paper, a mass matching tolerance of 1 amu is used. Under these conditions, mass maps created by fast atom bombardment **mass spectrometry** and matrix-assisted laser desorption time-of-flight would also be applicable. In cases where multiple matches are obsd. or verification of the **protein identification** is needed, tandem **mass spectrometry** sequencing can be used to establish sequence similarity.

L35 ANSWER 44 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:644768 HCAPLUS
DOCUMENT NUMBER: 119:244768
TITLE: Rapid indentification of proteins by **peptide** **-mass** fingerprinting. [Erratum to document cited in CA119(15):155221x]
AUTHOR(S): Pappin, D. J.; Hojrup, P.; Bleasby, A. J.
CORPORATE SOURCE: Protein Sequencing Lab., Imp. Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Curr. Biol. (1993), 3(7), 487
CODEN: CUBLE2; ISSN: 0960-9822
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The errors were not reflected in the abstr. or the index entries.

L35 ANSWER 45 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:555221 HCAPLUS
DOCUMENT NUMBER: 119:155221
TITLE: Rapid indentification of proteins by **peptide** **-mass** fingerprinting
AUTHOR(S): Pappin, D. J. C.; Hojrup, P.; Bleasby, A. J.
CORPORATE SOURCE: Protein Sequencing Lab., Imp. Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Curr. Biol. (1993), 3(6), 327-32
CODEN: CUBLE2; ISSN: 0960-9822
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors report the development of the mol. wt. search (MOWSE)

peptide-mass database at the SERC Daresbury Lab. Practical experience showed that sample proteins can be **identified** uniquely from as few as 3 or 4 exptl. detd. peptide masses when these are screened against a fragment database that is derived from >50,000 proteins. **Peptide-mass** fingerprints can prove as discriminating as linear peptide sequences but can be obtained in a fraction of the time using less protein. In many cases, this allows for a rapid **identification** of a sample protein before committing it to protein sequence anal. Fragment masses also provide information, at the protein level, that is complementary to the information provided by large-scale DNA sequencing or mapping projects.

L35 ANSWER 46 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:58326 HCAPLUS
DOCUMENT NUMBER: 114:58326
TITLE: Strategies for determination of disulfide bridges in **proteins** using plasma desorption **mass spectrometry**
AUTHOR(S): Soerensen, Hans Holmegaard; Thomsen, Johannes; Bayne, Stephen; Hoejrup, Peter; Roepstorff, Peter
CORPORATE SOURCE: Novo Nordisk A/S, Gentofte, DK-2820, Den.
SOURCE: Biomed. Environ. Mass Spectrom. (1990), 19(11), 713-20
CODEN: BEMSEN; ISSN: 0887-6134
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Disulfide bridges have been assigned in 3 different **proteins** by locating possible disulfide-linked **peptides** in enzymic digests of the **proteins** based on their mol. wt. detd. by plasma desorption **mass spectrometry**. Different strategies have been employed including in situ redn. of the nitrocellulose-bound **peptides** and confirmation of **peptide identify** by Me esterification reactions or Edman degrdn. The latter was needed for **identification** of glycosylated disulfide-linked **peptides**. For insulins cleavaged between cysteine residues in close proximity was not possible; but a combination of mol. mass information, enzymic cleavage with 2 different enzymes and sequence anal. including **identification** of diphenylthiohydantoin-cystine could ensure an unambiguous assignment of the disulfide bridges.

L35 ANSWER 47 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1987:632347 HCAPLUS
DOCUMENT NUMBER: 107:232347
TITLE: Structural analysis of **glycoproteins**: **identification** of carbohydrates and other posttranslational modifications by **mass spectrometry**
AUTHOR(S): Carr, Steven A.; Roberts, Gerald D.
CORPORATE SOURCE: Dep. Anal., Phys. Struct. Chem., SmithKline and French Lab., Swedeland, PA, 19479, USA
SOURCE: Methods Protein Sequence Anal., [Proc. Int. Conf.], 6th (1987), Meeting Date 1986, 423-36. Editor(s): Walsh, Kenneth A. Humana: Clifton, N. J.
CODEN: 56DFAZ
DOCUMENT TYPE: Conference; General Review

LANGUAGE: English
AB A review with 33 refs. about some of the unique problems assocd. with structural characterization of **glycoproteins** and an anal. strategy utilizing fast-atom-bombardment **mass spectrometry** and biochem. manipulations for **identifying** sites of attachment of asparagine-linked carbohydrates, detg. the extent of glycosylation at specific sites and defining the compn. and heterogeneity of oligosaccharides from unique sites.

L35 ANSWER 48 OF 48 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1982:100377 HCAPLUS
DOCUMENT NUMBER: 96:100377
TITLE: 252Californium plasma desorption mass spectrometry
AUTHOR(S): Macfarlane, Ronald D.
CORPORATE SOURCE: Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA
SOURCE: Biomed. Mass Spectrom. (1981), 8(9), 449-53
CODEN: BMSYAL; ISSN: 0306-042X
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB The basic principles of 252Cf plasma desorption mass spectrometry are presented, with examples of its application including the **identification** of nonvolatile marine toxins (including the red tide toxin). A new variation in mass spectrometry, a study of time-dependent effects, is presented; it is a technique which can be used to follow dynamic changes as a result of chem. reactions occurring in a sample at room temp. This is possible in 252Cf plasma desorption mass spectrometry because the sample is conserved during the anal.

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=> d stat que
L4      2842848 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR AMIN? OR PROTEOME?)

L5       224579 SEA FILE=HCAPLUS (MASS(W)SPECTR?)
L6        26790 SEA FILE=HCAPLUS L4(L)L5
L14     1924052 SEA FILE=HCAPLUS (?PROTEIN? OR ?PEPTIDE? OR PROTEOME?)
L27        1886 SEA FILE=HCAPLUS L14 (W)MASS
L28        1074 SEA FILE=HCAPLUS L27 AND L6
L30         436 SEA FILE=HCAPLUS L28 AND IDENT?
L33        6258 SEA FILE=HCAPLUS L14(W)IDENT?
L34         115 SEA FILE=HCAPLUS L30 AND L33
L35          48 SEA FILE=HCAPLUS L34 NOT (2001 OR 2000 OR 1999)/PY
L36       18368 SEA FILE=HCAPLUS L14 AND L6
L38          93 SEA FILE=HCAPLUS L36 AND INDEX
L39          92 SEA FILE=HCAPLUS L38 NOT L35
L40          65 SEA FILE=HCAPLUS L39 NOT (2001 OR 2000 OR 1999)/PY
L41           4 SEA FILE=HCAPLUS L40 AND POLYPEPTIDE?
L44           4 SEA FILE=HCAPLUS L28 AND L38
L46           8 SEA FILE=HCAPLUS L41 OR L44


=> d ibib abs hitrn 146

L46 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2001 ACS
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ACCESSION NUMBER: 1997:584259 HCAPLUS
DOCUMENT NUMBER: 127:244507
TITLE: **Proteome** analysis of Spiroplasma melliferum (A56) and **protein** characterization across species boundaries
AUTHOR(S): Cordwell, Stuart J.; Basseal, David J.; Humphery-Smith, Ian
CORPORATE SOURCE: Center Proteome Research Gene-Product Mapping, National Innovation Center, Eveleigh, 1430, Australia
SOURCE: Electrophoresis (1997), 18(8), 1335-1346
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Spiroplasma melliferum (Class: Mollicutes) is a wall-less, helical bacterium with a genome of approx. 1460 kbp encoding 800 - 1000 gene-products. A two-dimensional electrophoresis gel ref. map of S. melliferum was produced by Phoretix 2-D gel software anal. of eight high quality gels. The ref. map showed 456 silver-stained and replicated **protein** spots. 156 **Proteins** (34% of visible **protein** spots) from S. melliferum were further characterized by one, or a combination, of the following: **amino** acid anal., **peptide-mass** fingerprinting via matrix assisted laser desorption ionization-time of flight (MALDI-TOF) **mass spectrometry**, and N-terminal **protein** microsequencing. **Proteins** with close relationships to those previously detd. from other species were identified across species barriers. Thus, this study represents the first larger-scale anal. of a **proteome** based upon the attribution of predominantly "unique numerical parameters" for **protein** characterization across species boundaries, as opposed to a sequence-based approach. This approach allowed all database entries to be screened for homol., as is currently the case for studies based on nucleic acid or **protein** sequence information. Several **proteins** studied from this organism were identified as hypothetical, or having no close homolog already present in the databases. Gene-products from major families such as glycolysis, translation, transcription, cellular processes, energy metab., and **protein** synthesis were identified. Several gene-products characterized in S. melliferum were not previously found in studies of the entire Mycoplasma genitalium and Mycoplasma pneumoniae (both closely related Mollicutes) genomes. The presence of such gene-products in S. melliferum is discussed in terms of genome size as compared with the smallest known free-living organisms. Finally, the levels of expression of S. melliferum gene-products were detd. with respect to total optical intensity assocd. with all visible **proteins** expressed in exponentially grown cells.

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L46 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1993:644768 HCAPLUS
DOCUMENT NUMBER: 119:244768
TITLE: Rapid indentification of **proteins** by

peptide-mass fingerprinting.
[Erratum to document cited in CA119(15):155221x]

AUTHOR(S): Pappin, D. J.; Hojrup, P.; Bleasby, A. J.
CORPORATE SOURCE: Protein Sequencing Lab., Imp. Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Curr. Biol. (1993), 3(7), 487
CODEN: CUBLE2; ISSN: 0960-9822
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The errors were not reflected in the abstr. or the **index** entries.

L46 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1991:20437 HCAPLUS
DOCUMENT NUMBER: 114:20437
TITLE: MacProMass: a computer program to correlate **mass spectral** data to **peptide** and **protein** structures
AUTHOR(S): Lee, Terry D.; Vemuri, Sunil
CORPORATE SOURCE: Div. Immunol., Beckman Res. Inst., City of Hope, Duarte, CA, 91010, USA
SOURCE: Biomed. Environ. Mass Spectrom. (1990), 19(11), 639-45
CODEN: BEMSEN; ISSN: 0887-6134
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A program known as MacProMass has been written for Macintosh computers to assist in the anal. of **mass spectral** data of **peptides** and **proteins**. The program employs a user friendly, graphical interface and accommodates a variety of **protein** structures including cyclic **peptides** and multiple chain **proteins**. In addn. to mol. mass calcns. for pos. and neg. mol. ions, MacProMass also calcs. elemental compn., **amino** acid compn., isoelec. point, surface free energy, and HPLC **index** values for whole structures and **peptide** fragments resulting from enzymic or chem. degrdn. Users can program their own **amino** acid residues and terminal groups. In addn. to search routines for both mass and sequence, theor. fragment ions for **peptide mass spectra** can be calcd. Anal. of variant **proteins** is facilitated with a subroutine that systematically catalogs single **amino** acid substitutions that correspond to mass differences between obsd. and expected mol. ions. Interchain and intrachain disulfide bonds and other types of linkages are maintained throughout the chem. and enzymic degrdn. operations.

L46 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1990:441319 HCAPLUS
DOCUMENT NUMBER: 113:41319
TITLE: Effects of **peptide** hydrophobicity and charge state on molecular ion yields in plasma desorption **mass spectrometry**
AUTHOR(S): Wang, Rong; Chen, Ling; Cotter, Robert J.
CORPORATE SOURCE: Sch. Med., Johns Hopkins Univ., Baltimore, MD, 21205, USA
SOURCE: Anal. Chem. (1990), 62(15), 1700-5

CODEN: ANCHAM; ISSN: 0003-2700
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Plasma desorption **mass spectra** were obtained for a series of **peptides**, grouped in 4 mass ranges having approx. 9, 20, 30, and 40 **amino** acid residues. Within each group, the individual **peptides** differed in hydrophobicity, charge state, and retention time, as measured on a reversed-phase HPLC column. Comparison of the mol. ion intensities in the pos. ion **mass spectra** of **peptides** from each group showed a strong dependence upon hydrophobicity and no correlation with charge state. Plasma desorption **mass spectra** of mixts. of all the **peptides** within each mass range generally resulted in the desorption of a single residue and suppression of the ion signal from other components. In most cases, this could be correlated with hydrophobicity, as calcd. from the Bull and Breese **index** (Bull, H.B.; Breese, K., 1974); however, a better correlation existed when the results were compared with reversed-phase retention times. In general, the spectra of mixts. were not influenced by charge state (except in the absence of hydrophobic **peptides**), as the same components in each **peptide** mixt. produced the most abundant ions in both pos. and neg. ion spectra.

L46 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1986:549134 HCAPLUS
DOCUMENT NUMBER: 105:149134
TITLE: An approach towards the complete FAB analysis of enzymic digests of **peptides** and **proteins**
AUTHOR(S): Naylor, Stephen; Findeis, A. Frederick; Gibson, Bradford W.; Williams, Dudley H.
CORPORATE SOURCE: Univ. Chem. Lab., Cambridge, CB2 1EW, UK
SOURCE: J. Am. Chem. Soc. (1986), 108(20), 6359-63
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A current limitation in the use of fast-atom-bombardment (FAB) **mass spectrometry** for mixt. anal. is that some components of the mixt., dissolved in matrixes such as glycerol, are not normally obsd. Three enzymic digestions (1 of a **polypeptide** and 2 of small **proteins**) were used to show that it is the hydrophilic **peptides** in a mixt. that are suppressed. By detn. of the FAB spectra of both pure hydrophilic and hydrophobic **peptides** and of mixts. of these, it is shown that (1) hydrophilic **peptides** alone give a relatively poor signal response and (2) hydrophilic **peptides** are further suppressed in the presence of hydrophobic **peptides** that initially occupy the surface of the matrix. A hydrophilicity/hydrophobicity **index** (.DELTA.F values) can be used to indicate which **peptide** may be suppressed. Suppression may be reduced by HPLC partial fractionation or the conversion of polar carboxyl groups to more hydrophobic ester derivs.

L46 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1984:2927 HCAPLUS

DOCUMENT NUMBER: 100:2927
TITLE: **Amino** acid sequence determination by gas chromatography-**mass spectrometry** of permethylated **peptides**. The application of capillary columns
AUTHOR(S): Rose, Keith; Bairoch, Amos; Offord, Robin E.
CORPORATE SOURCE: Dep. Biochim. Med., CMU, Geneva, 1211, Switz.
SOURCE: J. Chromatogr. (1983), 268(2), 197-206
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The application of capillary columns to the detn. of the **amino** acid sequence of **proteins** and **polypeptides** by gas chromatog.-**mass spectrometry** (GC-MS) of partial hydrolyzates is described and discussed for the case of the N.alpha.,.epsilon.-trifluoroacetyl-N,O-permethyl derivs. Retention indexes are detd. with the aid of a computer program. The **mass spectra** of methionine enkephalin obtained by GC-MS on a packed and on a capillary column are presented and a retention **index** calcd. Amts. of deriv. corresponding to subnanomole amts. of **peptides** are sufficient to provide full **amino** acid sequence information. To assist in the assignment of retention indexes above 4400, a mixt. of n-alkanes from a com. source was characterized by GC-MS up to n-C54H110, and was found to contain material up to an expected C72H146.

L46 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1976:474449 HCAPLUS
DOCUMENT NUMBER: 85:74449
TITLE: **Amino** acid sequencing by gas chromatography-**mass spectrometry** using trifluoro-dideuteroalkylated **peptide** derivatives. C. The primary structure of the carboxypeptidase inhibitor from potatoes
AUTHOR(S): Nau, Heinz; Biemann, K.
CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, Mass., USA
SOURCE: Anal. Biochem. (1976), 73(1), 175-86
CODEN: ANBCA2
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The carboxypeptidase inhibitor from potatoes was used to demonstrate the utility of gas chromatog.-**mass spectrometry** for the detn. of the primary structure of such large **polypeptides**. Two mixts. of **oligopeptide** fragments, obtained by limited acid hydrolysis and enzymic digestion of this **polypeptide**, were transformed into the corresponding mixts. of O-trimethylsilylated trifluoro-dideuteroethyl polyamino alcs. which were then analyzed by gas chromatog.-**mass spectrometry**. The resulting **mass spectral** and retention **index** data allowed the identification of 61 **oligopeptide** fragments that were assembled by the computer by positioning all 39 **amino** acid residues in a unique sequence (with the exception of the assignment of the primary amide groups of Asn and Gln).

L46 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2001 ACS
ACCESSION NUMBER: 1974:92814 HCAPLUS
DOCUMENT NUMBER: 80:92814
TITLE: Computer-assisted assignment of retention indexes in gas chromatography-mass spectrometry and its application to mixtures of biological origin
AUTHOR(S): Nau, H.; Biemann, K.
CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, Mass., USA
SOURCE: Anal. Chem. (1974), 46(3), 426-34
CODEN: ANCHAM
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A program was written for the automatic assignment of the retention indexes of all components eluted during a gas chromatog.-**mass spectrometry**-computer expt. A set of 3 std. compds. (e.g. n-alkanes) is conjected with the sample into the gas chromatograph. The computer then identifies these compds. by their **mass spectral** characteristics and uses their positions to assign retention indexes for the entire gas chromatogram. The combination of these 2 sets of data that are structure specific and complementary, namely retention indexes and **mass spectra**, constitutes a most efficient and reliable approach to the identification of compds. Applications to the identification of drugs in body fluids of comatose patients as well as to the complete characterization of **amino** acids and **oligopeptides** in derivatized **polypeptide** hydrolyzates are presented. The retention **index** data provided by this program can be used for manual interpretation as well as for computer-assisted interpretation and search system.